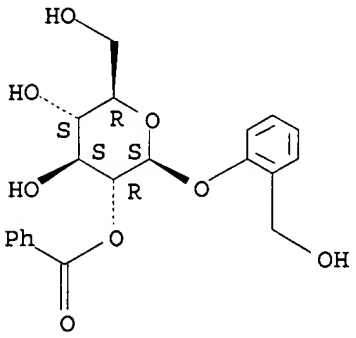
L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:634360 CAPLUS
DOCUMENT NUMBER: 117:234360
TITLE: Hemisynthesis of the naturally occurring tremuloidin
AUTHOR(S): Picard, Sophie; Bouyssou, Pascal; Chenault, Jacques
CORPORATE SOURCE: Lab. Chim. Bioorg. Anal. Assoc., Univ. Orleans, Orleans, F 45067, Fr.
SOURCE: Phytochemistry (1992), 31(8), 2909-10
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:234360

AB The hemisynthesis of tremuloidin under mild conditions by 2'-O-benzoylation of salicin is described. It appears as an essential step in synthesis of natural phenolic glycosides.

IT **529-66-8P**, Tremuloidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(**prepn**. of, from salicin)

RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:634360 CAPLUS
DOCUMENT NUMBER: 117:234360
TITLE: Hemisynthesis of the naturally occurring tremuloidin
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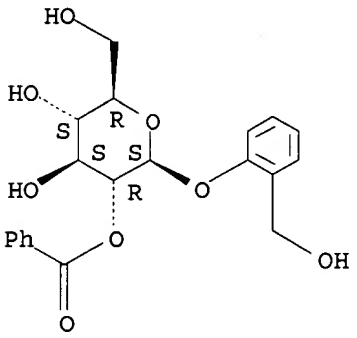
OTHER SOURCE(S): CASREACT 117:234360

AB The hemisynthesis of tremuloidin under mild conditions by 2'-O-benzoylation of salicin is described. It appears as an essential step in synthesis of natural phenolic glycosides.

IT **529-66-8P**, Tremuloidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(**prepn**. of, from salicin)

RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



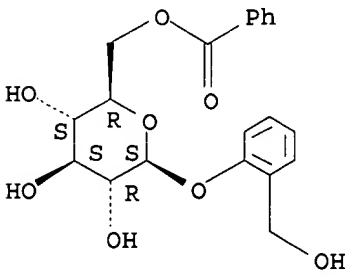
L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of Populus grandidentata
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **99-17-2**, Populin **138-52-3**, Salicin **529-66-8**, Tremuloidin
(in poplar leaves)

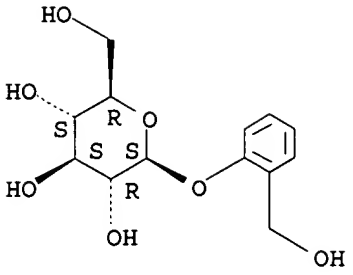
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



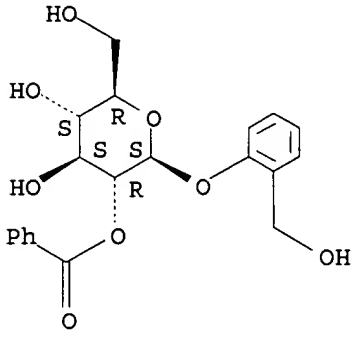
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



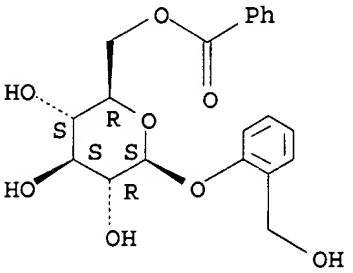
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **99-17-2**, Populin
(salicylate, in popular leaves)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

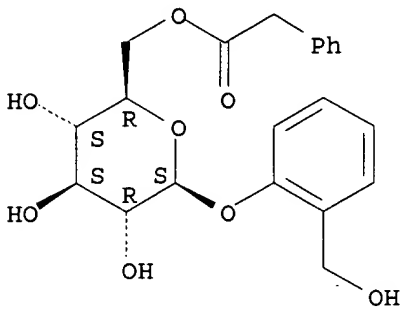
Absolute stereochemistry.



=> d scan

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
MF C21 H24 O8

Absolute stereochemistry.

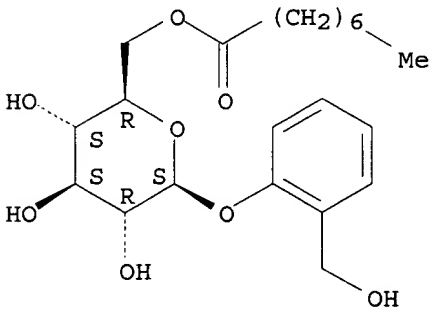


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-octanoate (9CI)
MF C21 H32 O8

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI)
MF C17 H24 O8

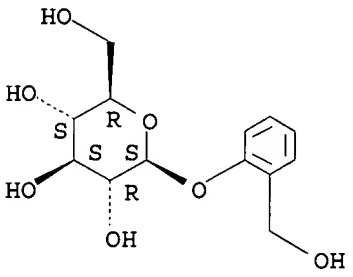
Absolute stereochemistry.

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:727039 CAPLUS
DOCUMENT NUMBER: 137:252711
TITLE: Melanin formation promoting agents containing salicylic acid or salicyl alcohol derivatives
INVENTOR(S): Hasegawa, Junichi; Tanaka, Kiyotaka
PATENT ASSIGNEE(S): Ichimaru Pharcos Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275060	A2	20020925	JP 2001-75402	20010316

PRIORITY APPLN. INFO.: JP 2001-75402 20010316
OTHER SOURCE(S): MARPAT 137:252711
AB The invention relates to a melanin formation promoting agent suitable for use in a cosmetic compn. for rough skin improvement and hair growth stimulation, etc., wherein the melanin formation promoting agent contains a salicylic acid or salicyl alc. deriv. A cosmetic emulsion contg. 2-**hydroxybenzoylaminoacetate** 0.1 % was prepd.
IT **138-52-3**
RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)
(melanin formation promoting agents contg. salicylic acid or salicyl alc. derivs.)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



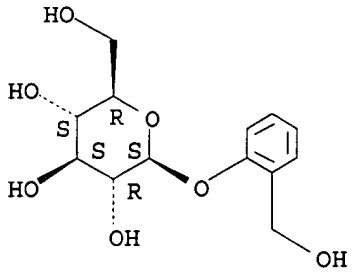
L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:468105 CAPLUS
DOCUMENT NUMBER: 119:68105
TITLE: Two phenolic glucosides and an iridoid glucoside from Alangium platanifolium var. trilobum
AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka
CORPORATE SOURCE: Kobe Women's Coll. Pharm., Kobe, 658, Japan
SOURCE: Phytochemistry (1993), 33(1), 161-4
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB From the leaves of Alangium platanifolium var. trilobum, two new phenolic glucosides, 7-O-methylsalicin and 7-O-(2,6-**dihydroxybenzoyl**)salicin, and a new iridoid glucoside, 7-O-benzoylloganic acid, were isolated and their structures detd. by spectroscopic and chem. studies. Six known compds. isolated for the first time from this plant were

identified as salicin, quercetin-3-O-.beta.-D-glucoside, rutin, adenosine, Me caffeate and roseoside.

IT **138-52-3**, Salicin **72021-23-9**, Henryoside
RL: BIOL (Biological study)
(from Alangium platanifolium trilobium)

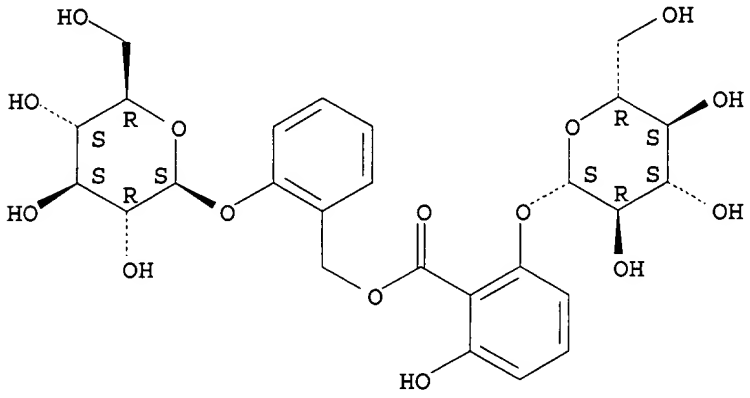
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 72021-23-9 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[[2-(.beta.-D-glucopyranosyloxy)-6-hydroxybenzoyl]oxy]methyl]phenyl (9CI) (CA INDEX NAME)

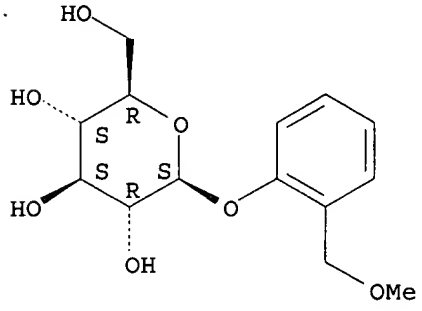
Absolute stereochemistry.



IT **148707-20-4 148707-21-5**
RL: BIOL (Biological study)
(isolation and structure of, from Alangium platanifolium trilobium)

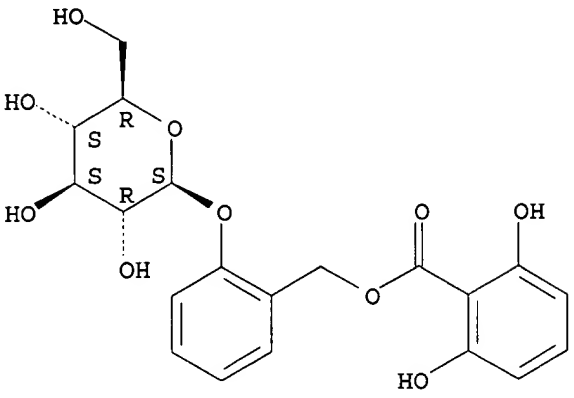
RN 148707-20-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(methoxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



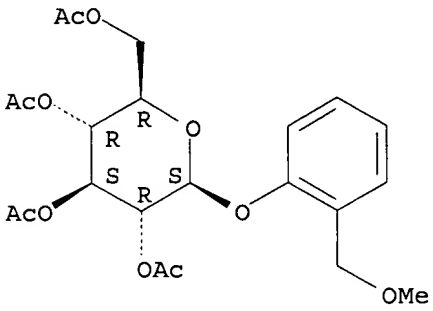
RN 148707-21-5 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[(2,6-dihydroxybenzoyl)oxy]methyl]phenyl (9CI) (CA INDEX NAME)

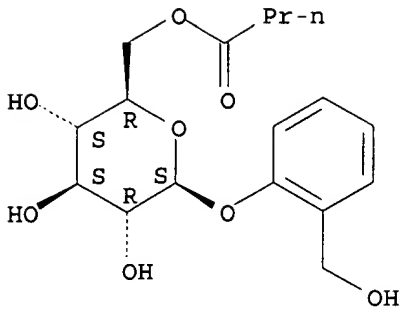
Absolute stereochemistry.



IT **148707-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 148707-23-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(methoxymethyl)phenyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



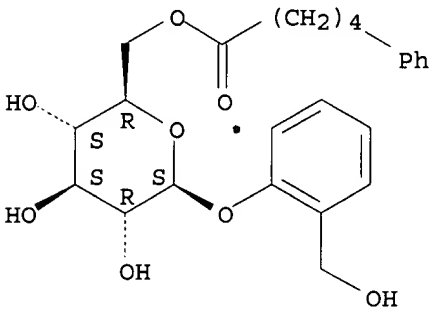


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenepentanoate (9CI)
MF C24 H30 O8

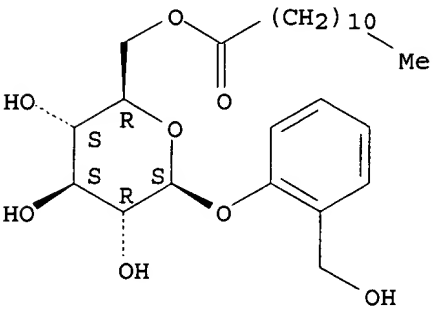
Absolute stereochemistry.

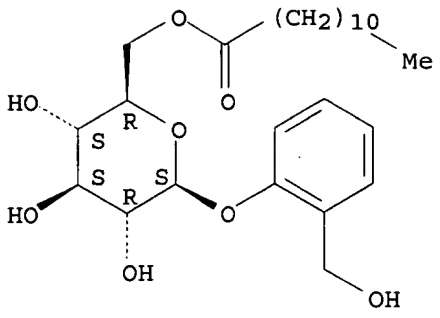


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-dodecanoate (9CI)
MF C25 H40 O8

Absolute stereochemistry.

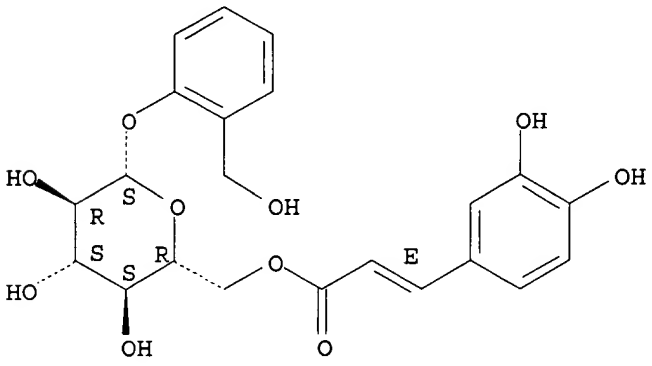




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

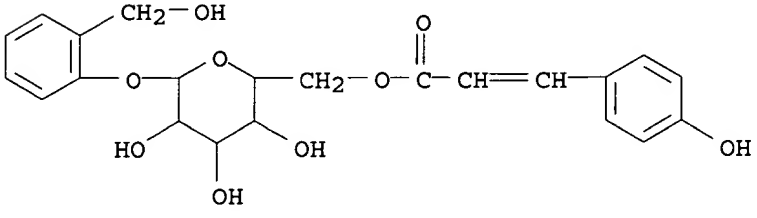
L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI)
MF C22 H24 O10

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

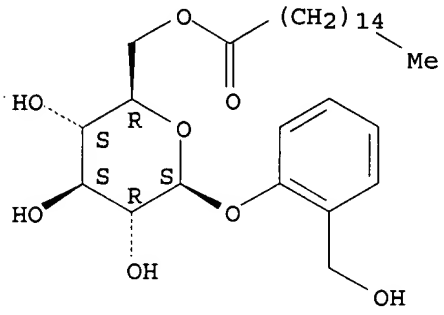
L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI)
MF C22 H24 O9



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-hexadecanoate (9CI)
MF C29 H48 O8

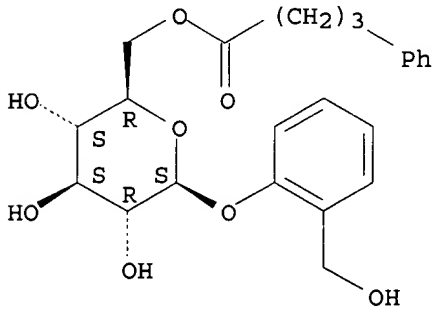
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI)
MF C23 H28 O8

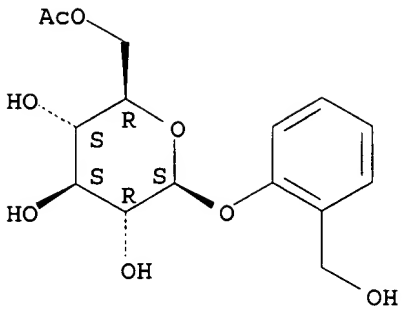
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI)
MF C15 H20 O8

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	141.42	141.63

FILE 'CAPLUS' ENTERED AT 13:01:55 ON 01 DEC 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 1 Dec 2002 VOL 137 ISS 23
FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d his

(FILE 'HOME' ENTERED AT 12:59:38 ON 01 DEC 2002)

FILE 'REGISTRY' ENTERED AT 12:59:46 ON 01 DEC 2002
L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 10 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:01:55 ON 01 DEC 2002

=> s l3

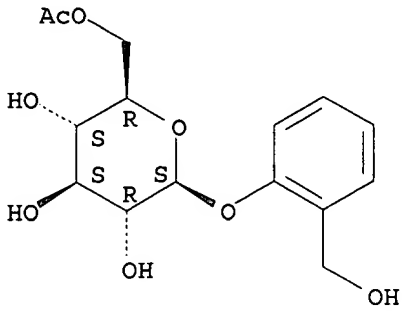
L4 26 L3

=> dup rem l4
PROCESSING COMPLETED FOR L4
L5 26 DUP REM L4 (0 DUPLICATES REMOVED)

=> d l4 1- ibib abs hitstr
YOU HAVE REQUESTED DATA FROM 26 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:363814 CAPLUS
DOCUMENT NUMBER: 137:198580
TITLE: Preferences of six leaf beetle species among qualitatively different leaf age classes of three Salicaceous host species
AUTHOR(S): Ikonen, Arsi
CORPORATE SOURCE: Department of Biology, University of Joensuu, Joensuu, FIN-80101, Finland
SOURCE: Chemoecology (2002), 12(1), 23-28
CODEN: CHMOE9; ISSN: 0937-7409
PUBLISHER: Birkhaeuser Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB As Salicaceous plants produce new leaves for a prolonged period of time, they expose a wide range of differentially aged leaves to herbivores during the growing season. In this work, it was shown that young leaves of three Salicaceous species, Populus tremula L., Salix phylicifolia L. and S. pentandra L., contain more nitrogen than conspecific old leaves. In P. tremula and S. pentandra young leaves also contained more low-mol. wt. secondary compds., phenolic glucosides. Leaves of S. phylicifolia did not contain phenolic glucosides in detectable amts. Furthermore, in P. tremula and S. pentandra young leaves contained less polymeric digestibility-reducing phenolics, condensed tannins, than old leaves. In S. phylicifolia, higher concns. of condensed tannins were found in young leaves. In lab. feeding trials with six leaf beetle species, young leaves of the studied plants were invariably preferred in all tested herbivore x host species combinations. In particular, it is remarkable that three leaf beetle species with known different overall relationships to phenolic glucosides equally preferred more glucoside-contg. young S. pentandra leaves over conspecific old ones. Four beetle species were found to prefer young leaves of S. phylicifolia despite the higher content of condensed tannins in young leaves. These results indicate that the general preference of leaf beetles for young leaves of Salicaceous plants probably does not primarily result from variable distribution of secondary compds. Apparently, the preference for young leaves is fundamentally due to variation in leaf nutritive traits, such as nitrogen content.
IT **19764-02-4**, Fragilin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(host preferences of leaf beetle species in relation to phenolic glucosides and differently aged leaves of Salicaceous host species)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:472959 CAPLUS
DOCUMENT NUMBER: 135:75834
TITLE: Enzyme-catalysed modification of substances in biological mixtures
INVENTOR(S): Otto, Ralf; Weiss, Albrecht
PATENT ASSIGNEE(S): Cognis Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046452	A1	20010628	WO 2000-EP12652	20001213
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 19962204	A1	20010705	DE 1999-19962204	19991222
EP 1240349	A1	20020918	EP 2000-987394	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

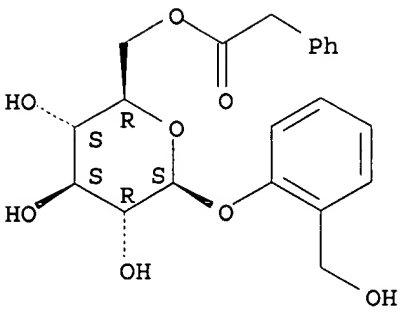
PRIORITY APPLN. INFO.: DE 1999-19962204 A 19991222
WO 2000-EP12652 W 20001213

AB The invention relates to an enzyme-catalyzed modification of substances in a mixt., comprising bringing the substance in a mixt. to be modified into contact with an enzyme and a substrate. Thus, arbutin present in a com. leaf ext. of bearberry was mixed with palmitic acid in the presence of an immobilized lipase and incubated at 45 .degree.C for 24 h. The resulting palmitoyl arbutin was then extd. with chloroform or methylene chloride.

IT **270081-79-3P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzyme-catalyzed modification of compds. in biol. exts.)

RN 270081-79-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

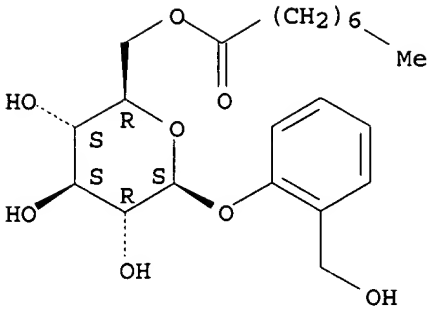
L4 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:155916 CAPLUS
DOCUMENT NUMBER: 132:344753
TITLE: Substrate specificity of lipase B from Candida antarctica in the synthesis of arylaliphatic glycolipids
AUTHOR(S): Otto, R. T.; Scheib, H.; Bornscheuer, U. T.; Pleiss, J.; Syldatk, C.; Schmid, R. D.
CORPORATE SOURCE: Institut fur Technische Biochemie, Universitat Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Journal of Molecular Catalysis B: Enzymatic (2000), 8(4-6), 201-211
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Arylaliph. glycolipids are known for their pharmaceutical and medicinal properties. We found that a great variety of arylaliph. esters can be synthesized from non-activated substrates such as glucose or the naturally-occurring drug salicin using lipase B from Candida antarctica (CAL-B). However, esters known to display anticancer activity such as those derived from arom. carboxylic acids or unsatd. arylaliph. acids, like cinnamic acid and its derivs., could not be obtained. In this work, along with syntheses of new glycolipids, we performed computer-aided mol. modeling based on data from our recently published work to examine why some substances are accepted by CAL-B while others are not. In order to elucidate the advantages and limitations of CAL-B in the synthesis of arom. glycolipids, we investigated arylaliph. acyl donor access to the lipase binding site along with steric interactions between the glucoside aglycons and residues of the alc. binding pocket.

IT **270081-72-6P 270081-75-9P 270081-77-1P 270081-79-3P 270081-81-7P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(mol. modeling provides insight into substrate specificity displayed by Candida antarctica lipase B in synthesis of arylaliph. glycolipids)

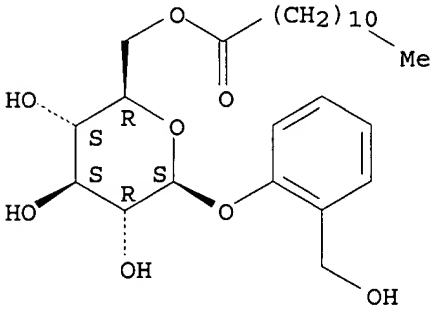
RN 270081-72-6 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-octanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



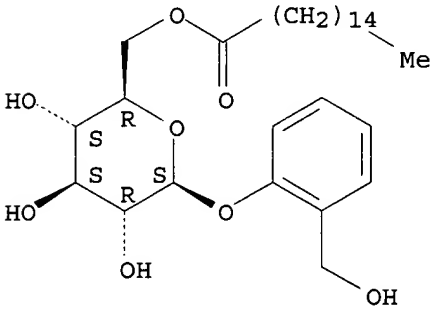
RN 270081-75-9 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-dodecanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



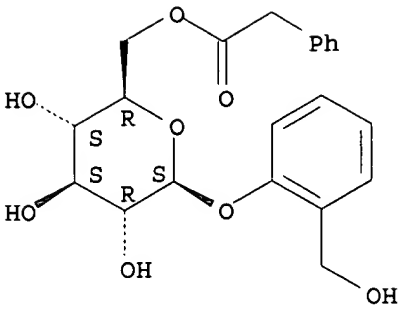
RN 270081-77-1 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-hexadecanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



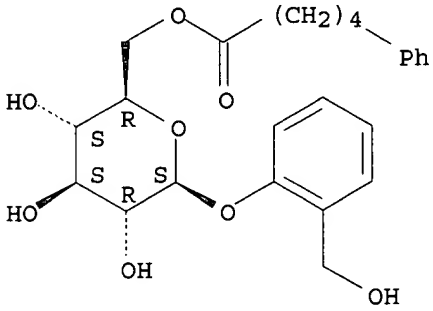
RN 270081-79-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 270081-81-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenepentanoate (9CI) (CA INDEX NAME)

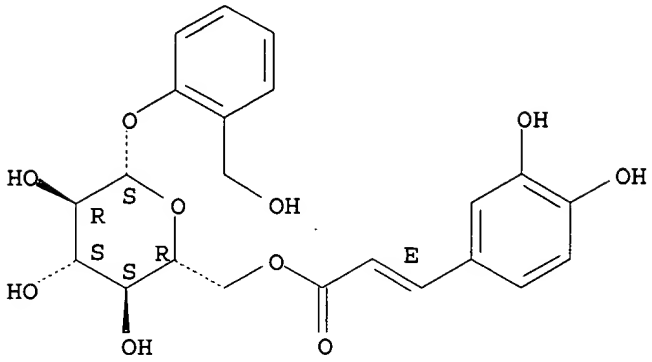
Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:799976 CAPLUS
DOCUMENT NUMBER: 132:134798
TITLE: Five Phenolic Glycosides from Alangium chinense
AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Ikejima, Sanae; Inoue, Miho; Nagakura, Naotaka; Inoue, Kenichiro; Kuwajima, Hiroshi; Wu, Hua-Xin
CORPORATE SOURCE: Kobe Pharmaceutical University, Higashinada-ku Kobe, 658-8558, Japan
SOURCE: Journal of Natural Products (2000), 63(1), 95-98
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB From the dried leaves of Alangium chinense, five novel phenolic glycosides, 6'-O-galloylsalicin, 4',6'-di-O-galloylsalicin, 4',6'-O-(S)-hexahydroxydiphenoylsalicin, 4',6'-O-(R)-hexahydroxydiphenoylsalicin, and pyrocatechol 1-O-.beta.-D-xylopyranosyl(1.fwdarw.6)-.beta.-D-glucopyranoside were isolated. The structures of these new compds. were detd. by spectroscopic methods.
IT **193280-04-5P**, 6'-O-trans-Caffeoylsalicin
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(phenolic glycosides from Alangium chinense)
RN 193280-04-5 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:393069 CAPLUS
DOCUMENT NUMBER: 131:43666
TITLE: Method for selective esterification of polyols
INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

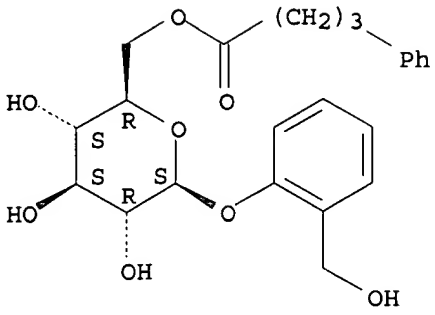
OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

IT **218966-96-2P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective esterification of polyols)

RN 218966-96-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



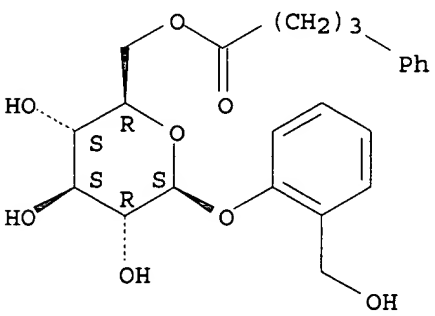
L4 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:708306 CAPLUS
DOCUMENT NUMBER: 130:80398
TITLE: Lipase-catalyzed synthesis of arylaliphatic esters of .beta.-D(+)-glucose, n-alkyl- and arylglucosides and characterization of their surfactant properties
AUTHOR(S): Otto, Ralf T.; Bornscheuer, Uwe T.; Syldatk, Christoph; Schmid, Rolf D.
CORPORATE SOURCE: Institut fur Bioverfahrenstechnik, Universitat Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Journal of Biotechnology (1998), 64(2,3), 231-237
CODEN: JBITD4; ISSN: 0168-1656
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

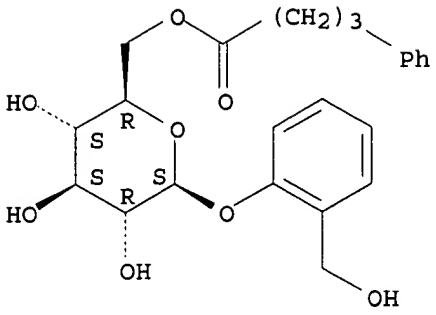
AB .beta.-D(+)-Glucose, n-alkyl-.beta.-D(+)-glucosides, salicin and 1-phenylglucoside were regioselectively acylated at the primary hydroxy group of the sugar moiety with a variety of non-activated arylaliph. carboxylic acids using lipase B from Candida antarctica in a mainly solid phase in the presence of a small amt. of t-butanol in yields up to 71%. The arylaliph. glucose esters were highly water sol. (15 to 100 g l-1) and showed surface activity. Crit. micellar concns. between 2 and 95 mM and minimal surface tensions around 35-45 mN m-1 were detd. The hydrophilic-lipophilic balance values of arylaliph. esters from .beta.-D(+)-glucose indicate a use in oil-in-water emulsions or detergents, whereas the n-alkyl- and arylglycosides can be employed as wetting agents or water-in-oil emulsifiers.

IT **218966-96-2P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(lipase-catalyzed synthesis of arylaliph. esters of .beta.-D(+)-glucose, n-alkyl- and arylglucosides and characterization of their surfactant properties)

RN 218966-96-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

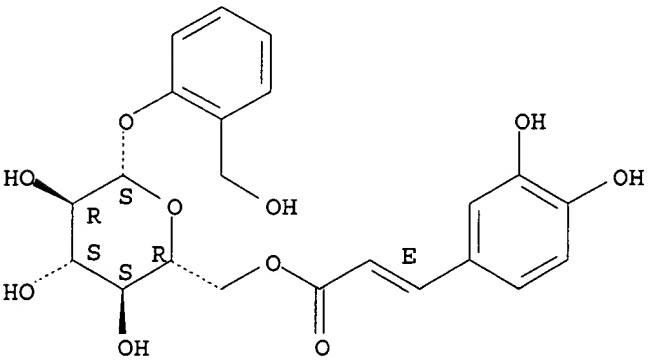




REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:505793 CAPLUS
DOCUMENT NUMBER: 127:147088
TITLE: Two new phenolic glycosides from Alangium chinense
AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka
CORPORATE SOURCE: Kobe Pharmaceutical University, Kobe, 658, Japan
SOURCE: Natural Medicines (Tokyo) (1997), 51(2), 173-175
CODEN: NMEDEO; ISSN: 1340-3443
PUBLISHER: Japanese Society of Pharmacognosy
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB From the leaves of Alangium chinense (LOUR.) HARMS, two novel glycosides, 6'-O-.beta.-D-xylopyranosylsalicin and 6'-O-trans-caffeoylsalicin, were isolated and their structures detd. on the basis of spectroscopic data.
IT **193280-04-5P**, 6'-O-trans-Caffeoylsalicin
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(phenolic glycosides from Alangium chinense)
RN 193280-04-5 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L4 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:668128 CAPLUS
DOCUMENT NUMBER: 125:323005
TITLE: Chemical studies on antituberculosis compounds from Salix capitata
AUTHOR(S): Keapigu, M. C.; Wang, Mingshi

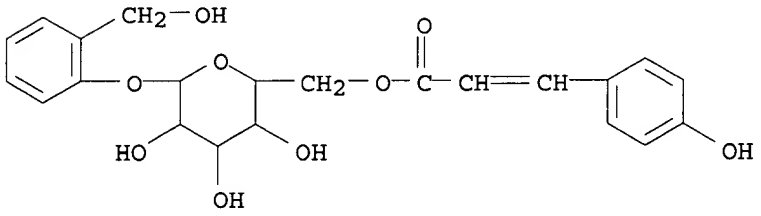
CORPORATE SOURCE: Dep. of Phytochemistry, China pharmaceutical Univ., Nanjing, 210009, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1996), 27(5), 271-273
CODEN: ZHYXE9; ISSN: 1000-5048
PUBLISHER: Zhongguo Yaoke Daxue
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ten constituents were isolated from the tender leaves of S. capitate, and identified as .beta.-sitosterol, stigmasterol, p-hydroxystyrene, cinnamic acid, salicyl alc., pyrocatechol, protocatechuic acid, daucosterol, salicin, and trichocarposide. P-hydroxystyrene was effective in inhibiting human mycobacterium tuberculosis. The structure of trichocarposide was cor. according to the exptl. data.

IT **17063-94-4**, Trichocarposide
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antituberculosis compds.from Salix capitata)

RN 17063-94-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:652067 CAPLUS
DOCUMENT NUMBER: 115:252067
TITLE: Extractive substances of bast, ligneous tissue, and fiber of flax straw
AUTHOR(S): Karpunin, I. I.; Murashkevich, T. V.
CORPORATE SOURCE: Beloruss NII Lenu, USSR
SOURCE: Vestsi Akademii Navuk BSSR, Seryya Khimichnykh Navuk (1991), (2), 59-64
CODEN: VBSKAK; ISSN: 0002-3590
DOCUMENT TYPE: Journal
LANGUAGE: Belorussian

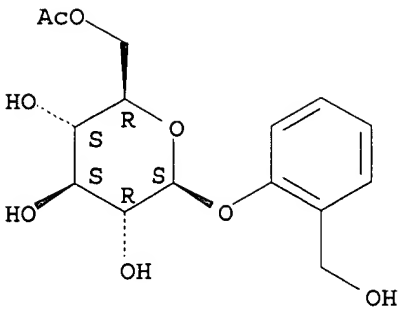
AB Glycosides and flavonols were lower in flax fiber than in the ligneous tissue and bast. Anthocyanins were high in the bast and low in the ligneous tissue and fiber. A bast constituent, 5,7,4-trihydroxyflavanone-5-(6-o-p-coumaroyl)glucopyranoside, known formerly from Salix bark, was identified for the first time in flax.

IT **19764-02-4**, Fragilin
RL: BIOL (Biological study)
(of flax straw fractions)

RN 19764-02-4 CAPLUS

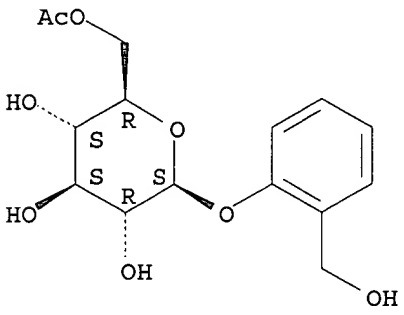
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:18845 CAPLUS
DOCUMENT NUMBER: 112:18845
TITLE: Phenolic constituents of Salix: a chemotaxonomic survey of further Finnish species
AUTHOR(S): Julkunen-Tiitto, R.
CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, 80101, Finland
SOURCE: Phytochemistry (1989), 28(8), 2115-25
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Various parts of some 30 Salix (willow) species were screened for 14 simple phenolic glucosides and salicyl alc. Species-specific qual. and quant. variation of phenolic glucosides in willow species was considerable and dependent on the part of the plant examd. Generally, there was greater diversity in glucoside compn. and a higher total amt. of glucosides in the twigs than in the leaves and buds. The traditional classification turned out to be inconsistent with a classification based on phenolic glucosides only. However, simple phenolic glucosides can be used for the recognition of exomorphol. similar species and hybrid forms. Salicyl alc. was not detected in any of the willow exts.
IT **19764-02-4**, Fragilin
RL: BIOL (Biological study)
(of Salix species, chemotaxonomy in relation to)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:406459 CAPLUS
DOCUMENT NUMBER: 111:6459
TITLE: Carbon-nutrient balance hypothesis in within-species phytochemical variation of Salix lasiolepis
AUTHOR(S): Price, Peter W.; Waring, Gwendolyn L.;

Julkunen-Tiitto, Riitta; Tahvanainen, Jorma; Mooney, Harold A.; Craig, Timothy P.

CORPORATE SOURCE: Dep. Biol. Sci., North. Arizona Univ., Flagstaff, AZ, 86011, USA

SOURCE: Journal of Chemical Ecology (1989), 15(4), 1117-31
CODEN: JCECD8; ISSN: 0098-0331

DOCUMENT TYPE: Journal

LANGUAGE: English

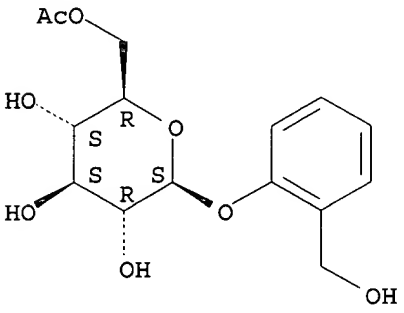
AB Predictions of the carbon-nutrient balance hypothesis were tested using a study of within-species phytochem. variation of the arroyo willow, S. lasiolepis. The prediction that a balance between nutrients (total protein) and carbon-based secondary metabolites (total phenols) should exist was supported using water treatment and fertilizer expts. and wild willow clones. Leaf nitrogen content and net photosynthetic rates of plants potted in soil in which parental plants grew was low, indicating that wild plants exist under relatively low nutrient status-high carbon balance conditions. The hypothesis also correctly predicted pos. relationships between shoot length and phenols in glasshouse plants, wild plants, and plants in the water treatment expt. and neg. relationships between shoot length and phenols in the fertilizer treatment expt. Total phenolic glycosides, fragilin, picetin, salicortin, tremulacin, and tremuloidin all correlated pos. with shoot length in glasshouse plants on a carbon-biased balance, and male willows had generally lower levels of phenolic glycosides than females. Salicortin and tremulacin showed the strongest pos. relationships with shoot length.

IT **19764-02-4**
RL: BIOL (Biological study)
(of Salix lasiolepis, shoot length in relation to)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:403512 CAPLUS

DOCUMENT NUMBER: 111:3512

TITLE: The effect of the sample preparation method of extractable phenolics of Salicaceae species

AUTHOR(S): Julkunen-Tiitto, R.; Tahvanainen, J.

CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101, Finland

SOURCE: Planta Medica (1989), 55(1), 55-8
CODEN: PLMEAA; ISSN: 0032-0943

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of different tissue prehandling methods on the phenolic content of willow bark, leaves, and twigs was studied. The phenolics were extd. at room temp., purified, and analyzed by high-resoln. capillary gas chromatog. Neither oven drying at a low temp. nor room drying of fresh leaves and oven drying of bark produced any qual. changes in the glucoside

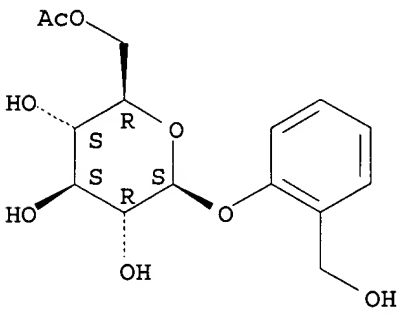
compn. and only a minor binding effect was seen on the amts. of each glucoside. On the other hand, oven drying of the intact long twigs and room drying of the bark are prehandling methods to avoid. Freeze drying or immediate anal. of frozen leaves lowered the total amt. of glucosides and caused considerable qual. changes to the glucoside compn. Acetone (80%) was a slightly more effective and gentle extn. solvent for all glucosides compared with methanol.

IT **19764-02-4**, Fragilin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in willow by gas chromatog., sample prepn. method effect on)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:489072 CAPLUS

DOCUMENT NUMBER: 109:89072

TITLE: Comparative high-performance liquid and gas-liquid chromatographic determination of phenolic glucosides in Salicaceae species

AUTHOR(S): Meier, B.; Julkunen-Tiitto, R.; Tahvanainen, J.; Sticher, O.

CORPORATE SOURCE: Dep. Pharm., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.

SOURCE: Journal of Chromatography (1988), 442, 175-86
CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

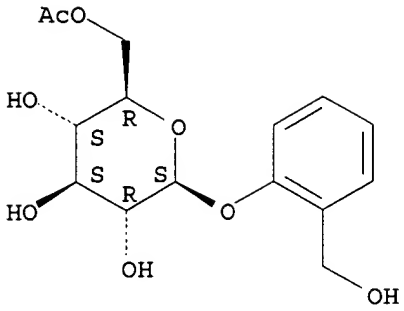
AB The phenolic glucosides of 7 willow species with different glucoside patterns were extd., purified, and analyzed by GC and HPLC. Two sample prepn. methods were used. It was shown that the HPLC and GC methods give comparable qual. and quant. results for the phenolic glucoside contents of the tested willows. Consequently, both methods can be used for species-specific screening of the glucoside patterns of Salicaceae species.

IT **19764-02-4**, Fragilin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in willow species by GC and HPLC)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

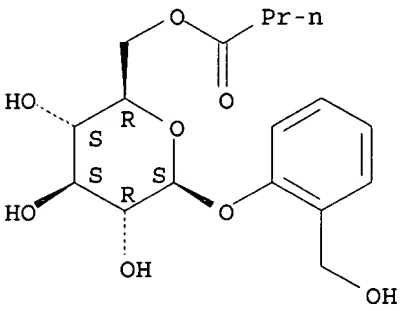


L4 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:52346 CAPLUS
DOCUMENT NUMBER: 108:52346
TITLE: Protease-catalyzed regioselective esterification of sugars and related compounds in anhydrous dimethylformamide
AUTHOR(S): Riva, Sergio; Chopineau, Joel; Kieboom, A. P. G.; Klibanov, Alexander M.
CORPORATE SOURCE: Dep. Appl. Biol. Sci., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1988), 110(2), 584-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By taking advantage of the unique dissolving potency of DMF and the broad substrate specificity of subtilisin, a no. of carbohydrates and other sugar-contg. compds. were regioselectively acylated via enzymic transesterification. Monobutyryl esters of the disaccharides maltose, cellobiose, lactose, and sucrose were prepd. readily on a gram scale. The presence of a bulky aglycon moiety does not substantially reduce the catalytic efficiency of subtilisin in DMF, thus permitting preparative enzymic esterification of natural compds. such as riboflavin, salicin, and the nucleosides adenosine and uridine. The reactivity of subtilisin only modestly drops upon an increase in the size of the carbohydrate substrate from maltose to maltoheptose. In addn. to the butyryl group, various N-acetylamino acid residues were enzymically introduced into sugars. Both highly purified and crude prepns. of subtilisin were used successfully as practical catalysts of transesterifications in dry DMF.

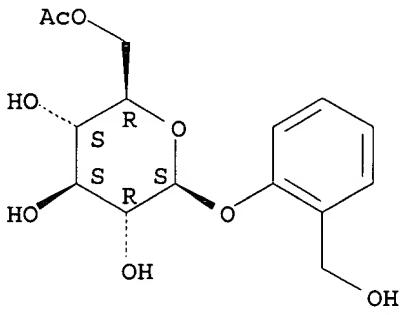
IT **111933-84-7P**
RL: PREP (Preparation)
(prepn. of, by esterification of subtilisin in anhyd. DMF)
RN 111933-84-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:34778 CAPLUS
DOCUMENT NUMBER: 108:34778
TITLE: Phenolics in the leaves and twigs of Salix pentandra L. (Salicaceae)
AUTHOR(S): Julkunen-Tiitto, R.
CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, Finland
SOURCE: Bulletin de Liaison - Groupe Polyphenols (1986), 13, 583-5
CODEN: BLPLAS; ISSN: 0242-8466
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The seasonal variations of phenolic glucosides (salicin, fragilin, picein, and salicortin) in leaves and twigs of S. pentandra are reported. The concn. of total phenolics in the leaves and current growth twigs continuously increased during the growing season reaching its highest value in mid-Sept.; before winter dormancy and leaf abscission a .apprx.50% drop in total phenolics occurred.
IT **19764-02-4**, Fragilin glycoside
RL: PROC (Process)
(in leaves and twigs of Salix pentandra, seasonal variation of)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

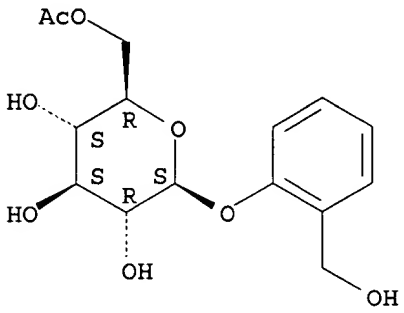
Absolute stereochemistry.



L4 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:218406 CAPLUS
DOCUMENT NUMBER: 102:218406
TITLE: Chemotaxonomical screening of phenolic glycosides in northern willow twigs by capillary gas chromatography
AUTHOR(S): Julkunen-Tiitto, R.
CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101/10, Finland
SOURCE: Journal of Chromatography (1985), 324(1), 129-39
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The phenolic glycosides in the twig tissues of willows and common aspen (Salicaceae) were extd., purified, and chromatographed using a SE-52 column. The glycosides screened were salicin, fragilin, picein, salidroside, vimalin, triandrin, tremuloidin, populin, salicortin, and grandidentatin. Each species exhibited a typical glycoside compn., which could change during the plant's life span. The glycosidic spectra may be used with certain reservations for the identification of unknown Salix and Populus species.
IT **19764-02-4**
RL: BIOL (Biological study)

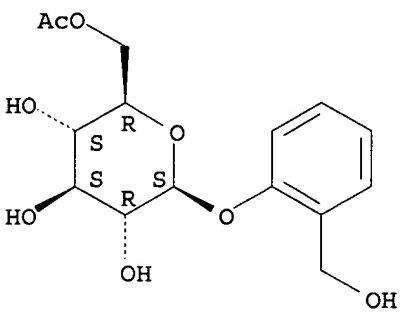
(of aspen and willow species, in twigs, taxonomy in relation to)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:156653 CAPLUS
DOCUMENT NUMBER: 78:156653
TITLE: Phenolic glycosides of Salix pentandroides roots
AUTHOR(S): Kompantsev, V. A.; Shinkarenko, A. L.
CORPORATE SOURCE: Pyatigorsk. Farm. Inst., Pyatigorsk, USSR
SOURCE: Khim. Prir. Soedin. (1973), 9(1), 126
CODEN: KPSUAR
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The fresh bark of 2-5-years-old S. pentandroides collected in June was extd. with EtOH-MeOH (1:1). The ext. was evapd. in vacuo, dild. with H2O, purified by extn. with CHCl3, pptd. with Pb subacetate, and the filtrate extd. with EtOAc. The cryst. glycoside obtained yielded on hydrolysis HOAc and salicin; it was identified as fragilin. After the removal of fragilin the EtOAc ext. was analyzed on a cellulose column. Fractional elution with BuOH-toluene-H2O (4:6:8) yielded (42-56th 50-ml fraction) salicin.
IT **19764-02-4**
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Salix pentandroides)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



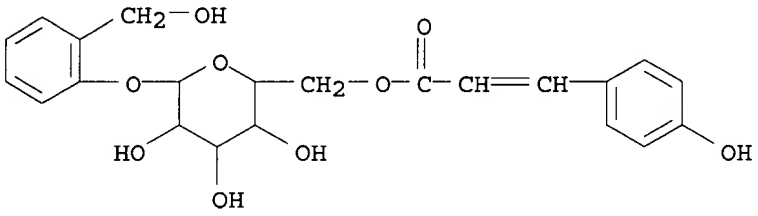
L4 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:61582 CAPLUS
DOCUMENT NUMBER: 74:61582
TITLE: Barks of the family Salicaceae. XXVI. Hot water extractives of the bark and leaves of Populus deltoides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. Paper Chem., Appleton, Wis., USA
SOURCE: Can. J. Chem. (1971), 49(1), 49-55
CODEN: CJCHAG
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The hot water extractives of the fresh smooth green bark and the fresh leaves of a P. deltoides tree cut in June and homogenized in EtOH were extd. fractionally with EtOAc, and the individual EtOAc exts. were fractionated by elution chromatog. with water, 20% EtOH, and 50% EtOH on polyamide columns. Important components found in the bark were salicortin, salicin, salicyl alc., pyrocatechol, .omega.-salicyloylsalicin, grandidentatin, grandidentoside, populoside, trichocarposide, and 6-methyldihydroquercetin. Important components found in the leaves were salicortin, salicin, salicyl alc., pyrocatechol, 1-O-p-coumaroyl-.beta.-D-glucoside, populoside, .omega.-salicyloylsalicin, chrysin-7-glucoside, and a new glucoside, deltoidin, which has been identified as 2-O-salicyloylsalicin.

IT **17063-94-4**
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Populus deltoides)

RN 17063-94-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)

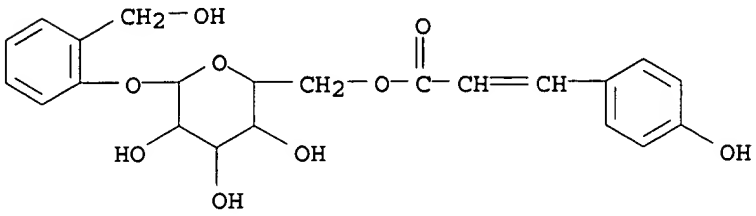


L4 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1970:97305 CAPLUS
DOCUMENT NUMBER: 72:97305
TITLE: Barks of the family Salicaceae. XXIII. Investigation of the hot-water extractives of Populus balsamifera bark
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA
SOURCE: Phytochemistry (1969), 8(12), 2393-6
CODEN: PYTCAS
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A no. of components were found in P. balsamifera bark which were not previously recorded from this important pulpwood species. These are salicortin, trichocarposide, populoside, salicyloylsalicin, and dihydromyricetin. A new procedure for chromatog. on polyamide columns gave a greater recovery than previously obtained.

IT **17063-94-4**
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Populus balsamifera)

RN 17063-94-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



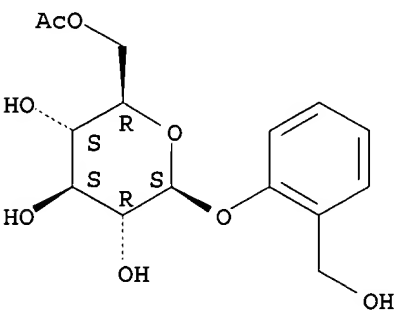
L4 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1970:18977 CAPLUS
DOCUMENT NUMBER: 72:18977
TITLE: Separation of phenolic glucosides by gel filtration
AUTHOR(S): Repas, A.; Nikolin, B.; Dursun, K.
CORPORATE SOURCE: Univ. Sarajevo, Sarajevo, Yugoslavia
SOURCE: J. Chromatogr. (1969), 44(1), 184-7
CODEN: JOCRAM
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The method of gel filtration was applied to the sepn. of more complex mixts. of naturally occurring phenolic glucosides. The freshly obtained bark of various Salicaceae species was extd. with 96% EtOH and the ext. was treated with an excess of basic lead acetat e. The mixt. was filtered, and Pb removed from the clear filtrate by treatment with H2S. The phenolic glucosides (10-15 mg sample in 2-3 ml eluent) were sepd. on Sephadex G-25 or Sephadex LH-20 by using water, H2O-EtOH (9:1), H2O-MeOH (9:1), or 96% EtOH as eluents and H2SO4 as the colorim etric reagent. The absorbance of the colored salicin-H2SO4 complex was max. at 510 m.mu.. The fractionated glucosides were identified by thin-layer chromatog. on silica gel in a CHCl3-MeOH (4:1) system. Salicin, populin, tremuloidin, salireposide, and grandidentatin were best sepd. on Sephadex G-25 with H2O-EtOH (9:1) or H2O-MeOH (9:1). In all cases, fragilin and triandrin were eluted simultaneously with salicin.

IT **19764-02-4**
RL: PROC (Process)
(sepn. of, by gel filtration)

RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2002 ACS

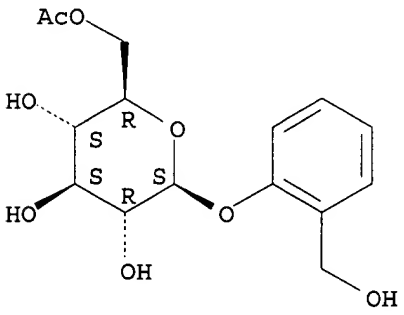
ACCESSION NUMBER: 1968:457517 CAPLUS
DOCUMENT NUMBER: 69:57517
TITLE: Phytochemistry of Salix species. I. A gas-liquid chromatographic procedure for the separation of phenolic glycosides
AUTHOR(S): Bolan, M.; Steele, J. W.
CORPORATE SOURCE: Sch. Pharm., Univ. Manitoba, Winnipeg, Manitoba, Can.
SOURCE: J. Chromatogr. (1968), 36(1), 22-30
CODEN: JOCRAM
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ten phenolic glycosides commonly found in Salix species were sepd. and identified by gas-liq. chromatog. of the trimethylsilyl ether derivs. The derivs. were prepd. by dissolving 0.01-0.05 mg. of pure glycoside or 0.1-0.3 mg. of natural or artificial mixts. in 50 .mu.l. Tri-Sil, shaking, and allowing the mixt. to stand 15 min. at room temp. before chromatog. He carrier gas, a flame ionization detector, and acid-washed, Me2SiCl2-treated column supports were used. All 10 glycosides were sepd. on a 0.5% cyclohexanedimethanol succinate/Chromosorb G column, although the peaks for salidroside (I) and fragilin (II) had overlapping bases. The glycoside and retention time relative to trimethylsilyl arbutin are, resp.: salicin (III), 0.64; I, 1.65; II, 1.75; picein (IV), 2.41; triandrin, 2.70; vimalin, 2.86; populin, 3.30; tremuloidin, 3.23; salireposide, 3.54; grandidentatin, 4.21. A 0.3% OV-1/Chromosorb G column completely resolved I. II was sepd. from all other components on a 0.2% OV-17/Chromosorb G column. A 1.5% diethylene glycol succinate (DEGS)/Chromosorb W column tended to cause some tailing of the peaks but was useful for obtaining addnl. evidence for the identification of admixed components and to check that no other separable components were present. III and IV were identified as the principle constituents of the trimethylsilylated cryst. fraction of a natural glycoside ext. by gas and chromatographic anal. on an OV-17 column and by ir and uv spectroscopy.

IT **19764-02-4**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, chromatographic)

RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

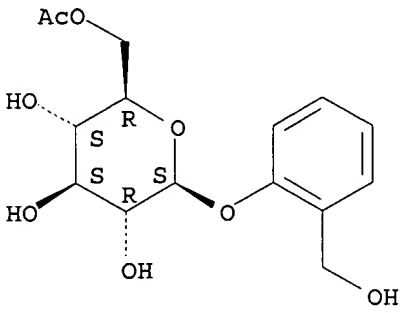
Absolute stereochemistry.



L4 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1968:454269 CAPLUS
DOCUMENT NUMBER: 69:54269
TITLE: Determination of phenolic glycosides in some domestic Salix species
AUTHOR(S): Kytkowska, Otylia
CORPORATE SOURCE: Inst. Lekow, Warsaw, Poland
SOURCE: Herba Pol. (1967), 13(4), 177-83
CODEN: HPBIA9

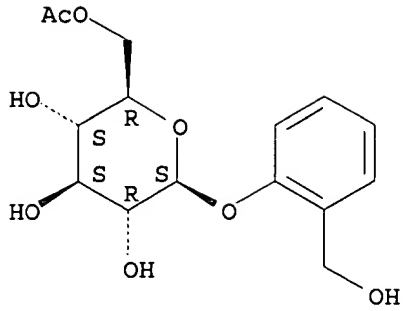
DOCUMENT TYPE: Journal
LANGUAGE: Polish
AB Combined EtOH and H2O exts. from barks of each of 7 Salix species (S. purpurea, S. alba, S. viminalis, S. caprea, S. cinerea, S. fragilis, and S. cordata) were evapd. in vacuo, extd. with EtOAc, and sepd. by paper chromatog. The samples contained salicin, triandrin, fragilin, salicortin, picein, vimalin, and salireposide. The triandrin levels were 0.45-5.35%, and those of salicortin, 0.05-4.8%.
IT **19764-02-4**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in Salix species)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

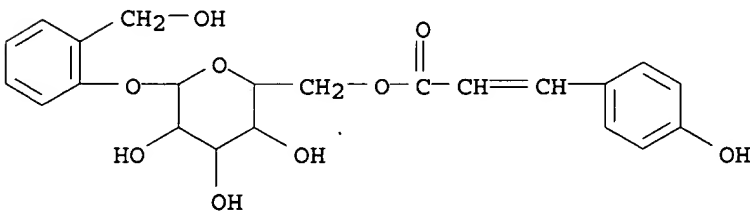


L4 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1968:436405 CAPLUS
DOCUMENT NUMBER: 69:36405
TITLE: The barks of the family Salicaceae. XV. The leaves of the family Salicaceae. 10. Mass spectrometry as an aid for determining structures of natural glucosides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA
SOURCE: Phytochemistry (1968), 7(5), 831-7
CODEN: PYTCAS
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Mass spectral fragmentation patterns were detd. for acetates of a no. of glucosides of unequivocally known structure which were isolated from the barks and leaves of trees of the family Salicaceae. All glucoside acetates, irrespective of size, indicated primary fragmentation at the C-1 bond, essentially similar to that found for completely acetylated glucose and methyl glucoside. In addn., the spectra of the acetates of glucosides with free phenolic groups demonstrated loss of acetyl as ketene either concurrently with or before the rupture of the C-1 bond. Presence or absence of ester substitution in the glucose moiety of the parent glucosides could thus be detd. with certainty, and possible location of substitution is indicated by relative intensities of fragment peaks.
IT **19764-02-4**
RL: PRP (Properties)
(mass spectrum of)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1967:514359 CAPLUS
DOCUMENT NUMBER: 67:114359
TITLE: Barks of the family Salicaceae. XIII. Hot-water extractives of the green bark of Populus trichocarpa
AUTHOR(S): Estes, Timothy K.; Pearl, Irwin A.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA
SOURCE: Tappi (1967), 50(7), 318-24
CODEN: TAPPAP
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 65: 9006c. The oven-dry ground bark of P. trichocarpa (1.5 kg.) was extd. with 20 l. hot H2O, the ext. filtered over Celite, and concd. in vacuo to .apprx.2 l. contg. 16% of the bark. The ext. was exhaustively extd. with CHCl3, Et2O, and EtOAc, giving the extractives I (8%), II (10%), and III (20%), resp. The final raffinate (IV) contained 62% of the hot H2O extractives. I was triturated with EtOH and the waxy residue discarded. I was then sepd. with Pb subacetate into 17% of a "Pb-sol." fraction, Ia, and 49% of a "Pb-insol." fraction, Ib. By polyamide chromatog. (P.C.) of Ia, salicin (V), salicyl alc. (VI), and tremuloidin (VII) and a mixt. of trichocarpin (VIII) and salireposide (IX) were isolated. P.C. of Ib indicated the presence of pyrocatechol, V, VI, VIII, and IX. Acid hydrolysis of I gave no salicyloylsalicin deriv. P.C. of II gave VIII, IX, p-coumaric acid (X), and trichocarposide (XI), m. 180-2.degree. (H2O), [.alpha.]20D -11.4.degree. (c 2.3, 80% Me2CO). Pb subacetate treatment of II gave VIII, IX, X, and XI. Pb subacetate and P.C. of II gave VIII, IX, X, and XI. Mild hydrolysis and P.C. of III indicated the presence of salicyloylsalicin-2 benzoate and X. P.C. of IV indicated the presence of glucose, fructose, and sucrose. Alk. hydrolysis of XI gave III and X; periodate oxidn. of XI consumed 2 moles with the liberation of 1 mole HCO2H. Hydrolysis of XI with .beta.-glucosidase gave no glucose. 21 references.
IT **17063-94-4**
RL: BIOL (Biological study)
(from Populus trichocarpa bark)
RN 17063-94-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)

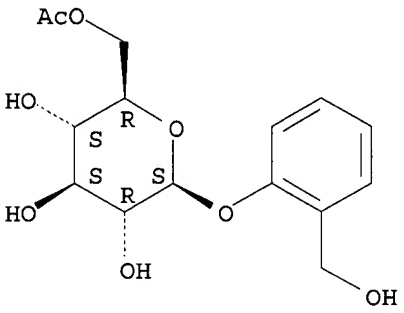


L4 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1964:462667 CAPLUS
DOCUMENT NUMBER: 61:62667
ORIGINAL REFERENCE NO.: 61:10918e-f
TITLE: Isolation of methoxyeugenol and trans-isoelemicin from the oil of nutmeg
AUTHOR(S): Shulgin, A. T.; Kerlinger, H. O.
CORPORATE SOURCE: Dow Chem. Co., Walnut Creek, CA
SOURCE: Naturwissenschaften (1964), 51(15), 360-1
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fractional distn. of oil of nutmeg gave 3 fractions. Fraction A cuts up to 114.degree. at 2 mm. consisted of terpenes, fraction B 114-119.degree. at 2 mm. contained myristicin (I) and elemicin (II), fraction C was a heavy oil residue which contained I and II as well as methoxyeugenol (III) and transisoelemicin (IV). Nuclear magnetic resonance, infrared, and mixed m.p. of the benzoate deriv. of III confirmed its identity. IV was confirmed by infrared anid its dibromo deriv. A search for trans-isomyristicin and the methoxylated analog revealed only extremely small traces.

IT **19764-02-4**, Salicin, 6'-acetate
(identity with fragilin from willow)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

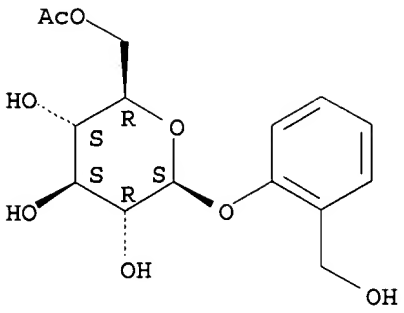


L4 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1964:462666 CAPLUS
DOCUMENT NUMBER: 61:62666
ORIGINAL REFERENCE NO.: 61:10918d-e
TITLE: The constitution of fragilin
AUTHOR(S): Thieme, H.
CORPORATE SOURCE: Univ. Leipzig, Germany
SOURCE: Naturwissenschaften (1964), 51(13), 310
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Fragilin (a new phenol-glucoside from Salix fragilis) was permethylated with MeI and Ag2O in dimethylformamide. Paper chromatographic examination showed the presence of 2,3,4-trimethylglucose, from which it was decided that fragilin is 6-acetylsalicin.

IT **19764-02-4**, Salicin, 6'-acetate
(identity with fragilin from willow)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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=> s l4 and esterification
          86110 ESTERIFICATION
            437 ESTERIFICATIONS
          86235 ESTERIFICATION
                  (ESTERIFICATION OR ESTERIFICATIONS)
L6            3 L4 AND ESTERIFICATION

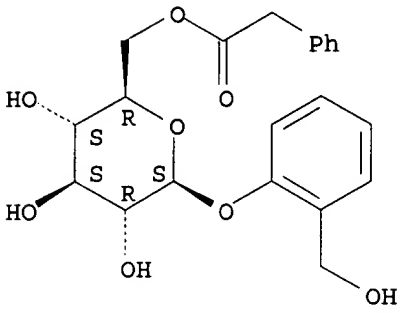
=> d l6 1- ibib abs hitstr
YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L6   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:         2001:472959  CAPLUS
DOCUMENT NUMBER:          135:75834
TITLE:                    Enzyme-catalysed modification of substances in
                          biological mixtures
INVENTOR(S):              Otto, Ralf; Weiss, Albrecht
PATENT ASSIGNEE(S):       Cognis Deutschland G.m.b.H., Germany
SOURCE:                   PCT Int. Appl., 26 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.         KIND  DATE           APPLICATION NO.  DATE
     ---------------    ----  --------       ---------------  --------
     WO 2001046452      A1    20010628       WO 2000-EP12652  20001213
         W:  JP, US
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, TR
     DE 19962204        A1    20010705       DE 1999-19962204 19991222
     EP 1240349         A1    20020918       EP 2000-987394   20001213
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI, CY, TR
PRIORITY APPLN. INFO.:                  DE 1999-19962204 A  19991222
                                        WO 2000-EP12652  W  20001213
AB   The invention relates to an enzyme-catalyzed modification of substances in
     a mixt., comprising bringing the substance in a mixt. to be modified into
     contact with an enzyme and a substrate.  Thus, arbutin present in a com.
     leaf ext. of bearberry was mixed with palmitic acid in the presence of an
     immobilized lipase and incubated at 45 .degree.C for 24 h.  The resulting
     palmitoyl arbutin was then extd. with chloroform or methylene chloride.
IT   270081-79-3P
     RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (enzyme-catalyzed modification of compds. in biol. exts.)
RN   270081-79-3  CAPLUS
CN   .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
```

(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:393069 CAPLUS
DOCUMENT NUMBER: 131:43666
TITLE: Method for selective **esterification** of polyols
INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

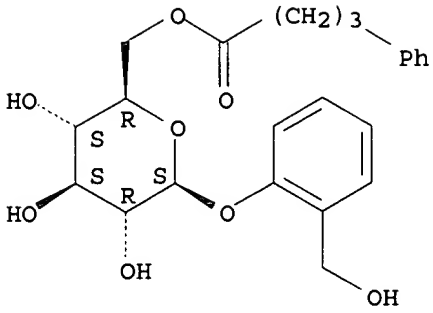
OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

IT **218966-96-2P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective **esterification** of polyols)

RN 218966-96-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

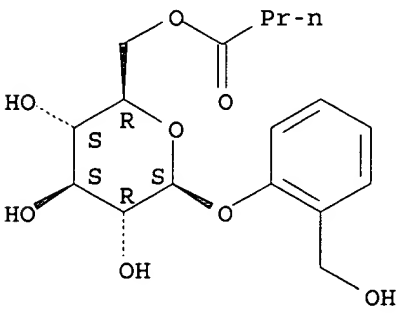


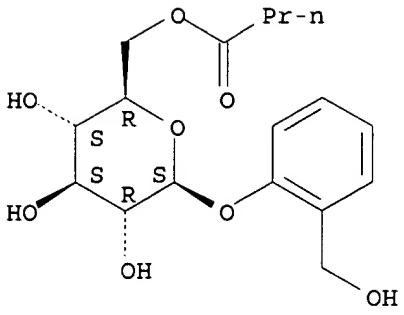
L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:52346 CAPLUS
DOCUMENT NUMBER: 108:52346
TITLE: Protease-catalyzed regioselective **esterification** of sugars and related compounds in anhydrous dimethylformamide
AUTHOR(S): Riva, Sergio; Chopineau, Joel; Kieboom, A. P. G.; Klibanov, Alexander M.
CORPORATE SOURCE: Dep. Appl. Biol. Sci., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1988), 110(2), 584-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By taking advantage of the unique dissolving potency of DMF and the broad substrate specificity of subtilisin, a no. of carbohydrates and other sugar-contg. compds. were regioselectively acylated via enzymic transesterification. Monobutyryl esters of the disaccharides maltose, cellobiose, lactose, and sucrose were prepd. readily on a gram scale. The presence of a bulky aglycon moiety does not substantially reduce the catalytic efficiency of subtilisin in DMF, thus permitting preparative enzymic **esterification** of natural compds. such as riboflavin, salicin, and the nucleosides adenosine and uridine. The reactivity of subtilisin only modestly drops upon an increase in the size of the carbohydrate substrate from maltose to maltoheptose. In addn. to the butyryl group, various N-acetylamino acid residues were enzymically introduced into sugars. Both highly purified and crude prepns. of subtilisin were used successfully as practical catalysts of transesterifications in dry DMF.

IT **111933-84-7P**
RL: PREP (Preparation)
(prepn. of, by **esterification** of subtilisin in anhyd. DMF)
RN 111933-84-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L3             10 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 13:01:55 ON 01 DEC 2002
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L5             26 DUP REM L4 (0 DUPLICATES REMOVED)
L6              3 S L4 AND ESTERIFICATION
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 s l4 and prostaglandin
         60913 PROSTAGLANDIN
         39884 PROSTAGLANDINS
         69447 PROSTAGLANDIN
                 (PROSTAGLANDIN OR PROSTAGLANDINS)
L7            1 L4 AND PROSTAGLANDIN

=> d l7 1 ibib abs hitstr

L7   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:         2001:472959  CAPLUS
DOCUMENT NUMBER:          135:75834
TITLE:                    Enzyme-catalysed modification of substances in
                          biological mixtures
INVENTOR(S):              Otto, Ralf; Weiss, Albrecht
PATENT ASSIGNEE(S):       Cognis Deutschland G.m.b.H., Germany
SOURCE:                   PCT Int. Appl., 26 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2001046452      A1   20010628       WO 2000-EP12652  20001213
         W:  JP, US
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, TR
     DE 19962204        A1   20010705       DE 1999-19962204 19991222
     EP 1240349         A1   20020918       EP 2000-987394   20001213
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI, CY, TR
PRIORITY APPLN. INFO.:                   DE 1999-19962204 A  19991222
                                         WO 2000-EP12652  W  20001213
AB   The invention relates to an enzyme-catalyzed modification of substances in
     a mixt., comprising bringing the substance in a mixt. to be modified into
     contact with an enzyme and a substrate.  Thus, arbutin present in a com.
     leaf ext. of bearberry was mixed with palmitic acid in the presence of an
     immobilized lipase and incubated at 45 .degree.C for 24 h.  The resulting
     palmitoyl arbutin was then extd. with chloroform or methylene chloride.
IT   270081-79-3P
     RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (enzyme-catalyzed modification of compds. in biol. exts.)
RN   270081-79-3  CAPLUS
CN   .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
     (CA INDEX NAME)

Absolute stereochemistry.
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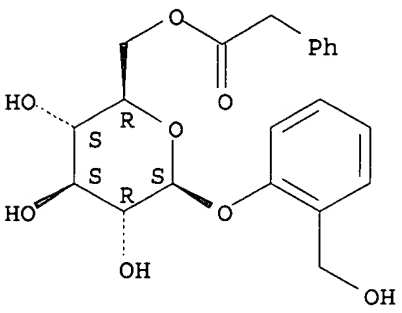

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REFERENCE COUNT:          11     THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> s l4 and inhibition of prostaglandin
         650067 INHIBITION
           4491 INHIBITIONS
         651545 INHIBITION
                  (INHIBITION OR INHIBITIONS)
          60913 PROSTAGLANDIN
          39884 PROSTAGLANDINS
          69447 PROSTAGLANDIN
                  (PROSTAGLANDIN OR PROSTAGLANDINS)
           2087 INHIBITION OF PROSTAGLANDIN
                  (INHIBITION(1W)PROSTAGLANDIN)
L8            0 L4 AND INHIBITION OF PROSTAGLANDIN

=> s l4 and prostaglandin(w)synthesis
          60913 PROSTAGLANDIN
          39884 PROSTAGLANDINS
          69447 PROSTAGLANDIN
                  (PROSTAGLANDIN OR PROSTAGLANDINS)
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           5951 PROSTAGLANDIN(W)SYNTHESIS
L9            0 L4 AND PROSTAGLANDIN(W)SYNTHESIS
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L11 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:403512 CAPLUS
DOCUMENT NUMBER: 111:3512
TITLE: The effect of the sample **preparation** method of extractable phenolics of Salicaceae species
AUTHOR(S): Julkunen-Tiitto, R.; Tahvanainen, J.
CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101, Finland
SOURCE: Planta Medica (1989), 55(1), 55-8
CODEN: PLMEAA; ISSN: 0032-0943
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect of different tissue prehandling methods on the phenolic content of willow bark, leaves, and twigs was studied. The phenolics were extd. at room temp., purified, and analyzed by high-resoln. capillary gas chromatog. Neither oven drying at a low temp. nor room drying of fresh leaves and oven drying of bark produced any qual. changes in the glucoside compn. and only a minor binding effect was seen on the amts. of each glucoside. On the other hand, oven drying of the intact long twigs and room drying of the bark are prehandling methods to avoid. Freeze drying or immediate anal. of frozen leaves lowered the total amt. of glucosides and caused considerable qual. changes to the glucoside compn. Acetone (80%) was a slightly more effective and gentle extn. solvent for all glucosides compared with methanol.

L11 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:489072 CAPLUS
DOCUMENT NUMBER: 109:89072
TITLE: Comparative high-performance liquid and gas-liquid chromatographic determination of phenolic glucosides in Salicaceae species
AUTHOR(S): Meier, B.; Julkunen-Tiitto, R.; Tahvanainen, J.; Sticher, O.
CORPORATE SOURCE: Dep. Pharm., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Journal of Chromatography (1988), 442, 175-86
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The phenolic glucosides of 7 willow species with different glucoside patterns were extd., purified, and analyzed by GC and HPLC. Two sample **prepn**. methods were used. It was shown that the HPLC and GC methods give comparable qual. and quant. results for the phenolic glucoside contents of the tested willows. Consequently, both methods can be used for species-specific screening of the glucoside patterns of Salicaceae species.

L11 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1970:78749 CAPLUS
DOCUMENT NUMBER: 72:78749
TITLE: Minor anthraquinones of Xanthoria parietina, the chlorination of parietin,, and the synthesis of **fragilin** and 7-chloroemodin ("AO-1")
AUTHOR(S): Sargent, Melvyn V.; Smith, David O'N.; Elix, J. A.
CORPORATE SOURCE: Univ. Chem. Lab., Canterbury, Engl.
SOURCE: J. Chem. Soc. C (1970), (2), 307-11
CODEN: JSOOAX
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Extn. of the lichen X. parietina yielded the anthraquinones emodin,teloschistin, and parietinic acid, as well as parietin (I). Chlorination of I with chlorine (1 mole) gave 5-chloroparietin, with chlorine (2 mole) gave chiefly 4,5-dichloroparietin, and with

excesschlorine gave 4,5,7-trichloroparietin (II). Dechlorination of II with excess sodium dithionite gave I and with a deficiency of sodium dithionite gave, after methylation, tri-O-methylemodin and 4,5,7-trichlorodi-O-methylparietin. Dechlorination of II with hydrazine hydrate and Pd/C after methylation, furnished di-O-methylfragilin III). Partial demethylation of III yielded **fragilin**, and complete demethylation of the former compd. afforded 7-chloroemodin.

L11 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1966:5478 CAPLUS
DOCUMENT NUMBER: 64:5478
ORIGINAL REFERENCE NO.: 64:1013c-d
TITLE: The phenolic glycosides of Salicaceae. V. Glycoside spectra and glycosidic content of Salix species of central Germany
AUTHOR(S): Thieme, Heinz
CORPORATE SOURCE: Karl Marx Univ., Leipzig, Germany
SOURCE: Pharmazie (1965), 20(9), 570-4
DOCUMENT TYPE: Journal
LANGUAGE: German
AB cf. CA 63, 11685g. Leaves, inflorescences, and barks of 11 willow spp. were studied, with sepn. wherever possible on the basis of sex. Paper chromatography, after preliminary purification of the exts. by passage through polyamide columns, was used to sep. the various glycosides isolated; they were identified by cochromatography or by elution and detn. of m.ps. or mixed m.ps. Glycosidal compn. was highly variable; salicin (I) (regarded as the chief glycoside of the Salicaceae) was detectable in all barks studied but was present only in small concns. and never was the chief glycoside. Larger amts. of acylated I derivs. were observed in various species; esp. high concns. of salicortin (II) or of triandrin were contained in barks of Salix purpurea or S. viminalis collected in mid-March. In contrast to the barks, leaves and inflorescences did not always contain phenol glycosides. The leaves of a few species; (S. myrsinifolia, S. purpurea, S. repens) evidenced noteworthy high concns. of I and II. No significant relation of glycoside content to sex of plant could be established. 27 references.

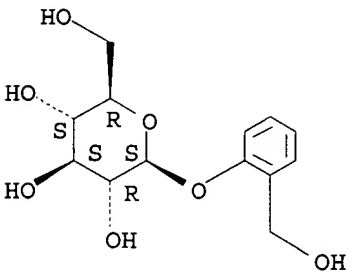
L11 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1965:438909 CAPLUS
DOCUMENT NUMBER: 63:38909
ORIGINAL REFERENCE NO.: 63:6930e-g
TITLE: The constitution of **fragilin**
AUTHOR(S): Bruun, Torger; Hollis, Donald P.; Ryhage, Ragnar
CORPORATE SOURCE: Norges Tek. Hogskole, Trondheim, Norway
SOURCE: Acta Chem. Scand. (1965), 19(4), 839-44
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB **Fragilin** (I) is a minor, colored constituent of the lichens Sphaerophorus fragilis (II) and S. coralloides. I was obtained from II and from S. globosus by extg. with ether for 24 hrs. The exts. were concd. and extd. successively with NaHCO3, Na2CO3, and NaOH. The org. material in the NaOH ext. was liberated with dil. H2SO4 and extd. with ether. After removal of the ether, an oil was recovered which gradually solidified and crystd. The crystals were isolated with ether or CHCl3 and purified by fractionated sublimation under reduced pressure and/or by crystn. from CHCl3, m. 267-8.degree.. Based on high resolution N.M.R. and mass spectroscopy, I was given the constitution below. The methoxy deriv. was obtained by methylation with Me2SO4 and K2CO3 in acetone, the yellow crystals were recovered from CHCl3-MeOH, m.p. 208-9.degree.. Acetylation with acetic anhydride in pyridine, overnight at room temp. yielded the acetate, the yellow crystals were recovered from acetone, m. 234-5.degree..

L5 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:727039 CAPLUS
DOCUMENT NUMBER: 137:252711
TITLE: Melanin formation promoting agents containing salicylic acid or **salicyl** alcohol derivatives
INVENTOR(S): Hasegawa, Junichi; Tanaka, Kiyotaka
PATENT ASSIGNEE(S): Ichimaru Pharcos Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275060	A2	20020925	JP 2001-75402	20010316

OTHER SOURCE(S): MARPAT 137:252711
AB The invention relates to a melanin formation promoting agent suitable for use in a cosmetic compn. for rough skin improvement and hair growth stimulation, etc., wherein the melanin formation promoting agent contains a salicylic acid or **salicyl** alc. deriv. A cosmetic emulsion contg. 2-hydroxybenzoylaminoacetate 0.1 % was prepd.
IT **138-52-3**
RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)
(melanin formation promoting agents contg. salicylic acid or **salicyl** alc. derivs.)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:521356 CAPLUS
DOCUMENT NUMBER: 137:75540
TITLE: Methods for generating doubled haploid maize plants
INVENTOR(S): Zheng, Yuanming; Konzak, Calvin F.; Weng, Yujia; Rafiullah, Sahibzada
PATENT ASSIGNEE(S): Northwest Plant Breeding Co., USA
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

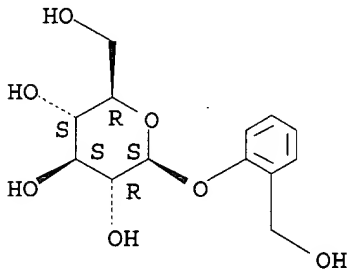
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2002052926 A2 20020711 WO 2002-US327 20020102
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2001-260028P P 20010105

AB In one aspect, the present invention provides methods for generating doubled haploid and/or haploid maize plants from microspores. The methods of this aspect of the invention include the steps of: (a) selecting maize plant material comprising maize microspores at a developmental stage amenable to androgenic induction; (b) incubating the microspores in incubation medium at a temp. and osmolarity effective to induce androgenesis to obtain temp.-treated microspores; (c) isolating the temp.-treated microspores; (d) cultivating the isolated, temp.-treated microspores in cultivation medium with either at least one live plant ovary and/or ovary-conditioned medium to produce regenerative maize tissue, wherein the cultivation medium has an osmolarity between about 300 mOsm and about 500 mOsm and comprises at least one cytokinin and at least one auxin; and (e) regenerating maize plants from the regenerative maize tissue. The present invention also provides methods for producing regenerative maize tissue from maize microspores.

IT **138-52-3**, Salicin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(methods for generating doubled haploid maize plants)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:405294 CAPLUS
DOCUMENT NUMBER: 137:43683
TITLE: Determination of triandrin and salicin in Salix viminalis L. by reversed-phase high-performance liquid chromatography
AUTHOR(S): Minakhmetov, R. A.; Onuchak, L. A.; Kurkin, V. A.; Zapesochnaya, G. G.; Medvedeva, S. A.
CORPORATE SOURCE: Department of Chemistry, Samara State University, Samara, 443011, Russia
SOURCE: Journal of Analytical Chemistry (Translation of Zhurnal Analiticheskoi Khimii) (2002), 57(4), 338-341
CODEN: JACTE2; ISSN: 1061-9348
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

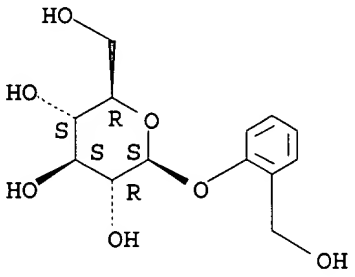
AB The optimal sepn. of phenolic components of the bark of basket willow Salix viminalis L. was attained using reversed-phase HPLC with isocratic elution. Triandrin (1-O-.beta.-D-glucopyranoside of p-coumaryl alc.) and salicin (1-O-.beta.-D-glucopyranoside of **salicyl** alc.) were identified. Regularities in the retention of triandrin and salicin in the Separon SGX C18-binary mobile phase (acetonitrile-H2O) system were considered. A procedure was developed for the quant. detn. of triandrin in raw basket-willow bark and its ext.

IT **138-52-3**, Salicin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of triandrin and salicin in Salix viminalis L. by reversed-phase high-performance liq. chromatog.)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:85522 CAPLUS

DOCUMENT NUMBER: 136:276441

TITLE: Functional expression of human liver cytosolic .beta.-glucosidase in Pichia pastoris. Insights into its role in the metabolism of dietary glucosides

AUTHOR(S): Berrin, Jean-Guy; McLauchlan, W. Russell; Needs, Paul; Williamson, Gary; Puigserver, Antoine; Kroon, Paul A.; Juge, Nathalie

CORPORATE SOURCE: Nutrition, Health and Consumer Sciences Division, Institute of Food Research, Norwich, NR4 7UA, UK

SOURCE: European Journal of Biochemistry (2002), 269(1), 249-258
CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

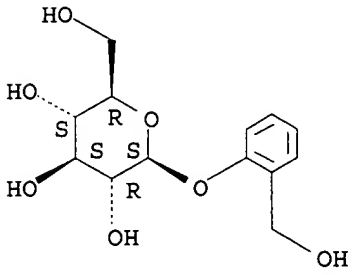
AB Human tissues such as liver, small intestine, spleen and kidney contain a cytosolic .beta.-glucosidase (CBG) that hydrolyzes various .beta.-D-glycosides, but whose physiol. function is not known. Here, we describe the first heterologous expression of human CBG, a system that facilitated a detailed assessment of the enzyme specificity towards dietary glycosides. A full-length CBG cDNA (cbg-1) was cloned from a human liver cDNA library and expressed in the methylotrophic yeast Pichia pastoris at a secretion yield of .apprx.10 mg/L. The recombinant CBG (reCBG) was purified from the supernatant using a single chromatog. step and was shown to be similar to the native enzyme isolated from human liver in terms of phys. properties and specific activity towards 4-nitrophenyl-.beta.-D-glucoside. Furthermore, the reCBG displayed a broad specificity with respect to the glycone moiety of various aryl-glycosides (.beta.-D-fucosides, .alpha.-L-arabinosides, .beta.-D-glucosides, .beta.-D-galactosides, .beta.-L-xylosides,

.beta.-D-arabinosides), similar to the native enzyme. For the first time, we show that the human enzyme has significant activity towards many common dietary xenobiotics including glycosides of phytoestrogens, flavonoids, simple phenolics and cyanogens with higher apparent affinities (Km) and specificities (kcat/Km) for dietary xenobiotics than for other aryl-glycosides. These data indicate that human CBG hydrolyzes a broad range of dietary glucosides and may play a crit. role in xenobiotic metab.

IT **138-52-3**, Salicin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(functional expression of human liver cytosolic .beta.-glucosidase and its role in metab. of dietary glucosides in Pichia pastoris)

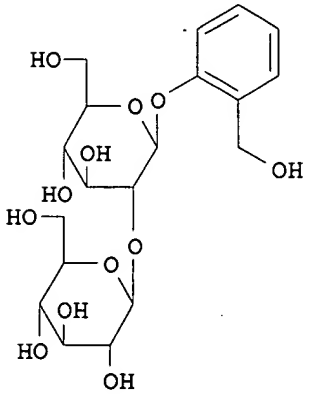
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:724753 CAPLUS
DOCUMENT NUMBER: 136:17988
TITLE: Glycosides of benzyl and **salicyl** alcohols from Alangium chinense
AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka; Inoue, Kenichiro; Kuwajima, Hiroshi; Wu, Hua-Xin
CORPORATE SOURCE: Kobe Pharmaceutical University, Kobe, 658-8558, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(10), 1343-1345
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



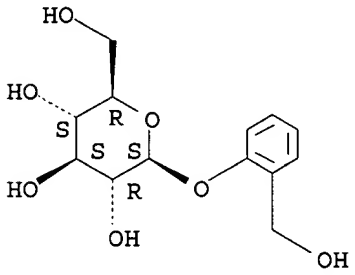
I

AB From the water-sol. fraction of the dried leaves of Alangium chinense, three new glycosides, benzyl alc. .beta.-D-glucopyranosyl-(1.fwdarw.2)-[.beta.-D-xylopyranosyl-(1.fwdarw.6)]-.beta.-D-glucopyranoside, 2'-O-.beta.-D-glucopyranosylsalicin (I), and 2'-O-.beta.-D-glucopyranosyl-6'-O-.beta.-D-xylopyranosylsalicin were isolated along with seven known glycosides. The structures of the new compds. were detd. by spectroscopic and chem. means.

IT **138-52-3**, Salicin **72021-23-9**, Henryoside
193280-03-4, 6'-O-.beta.-D-Xylopyranosylsalicin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(glycosides of benzyl and **salicyl** alcs. from Alangium chinense)

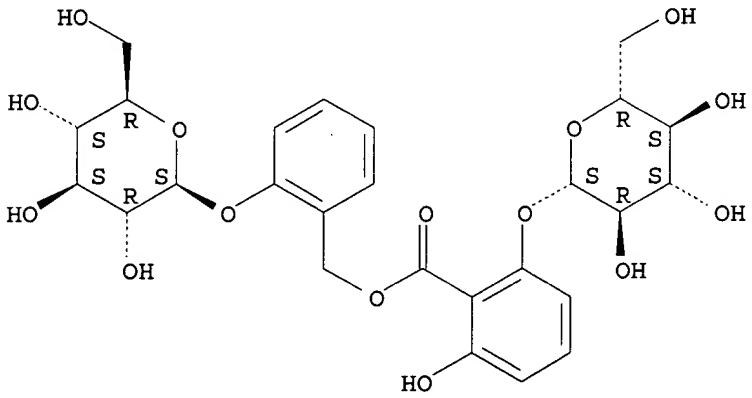
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



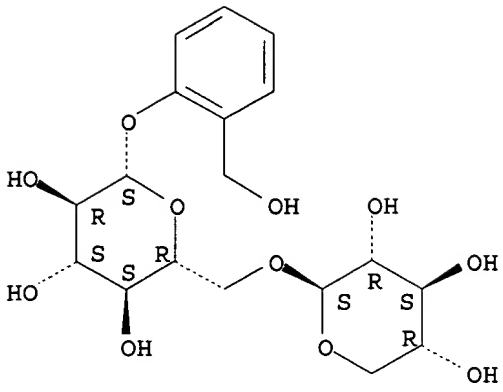
RN 72021-23-9 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[[2-(.beta.-D-glucopyranosyloxy)-6-hydroxybenzoyl]oxy]methyl]phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



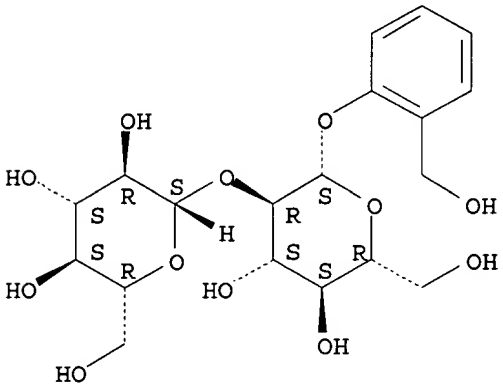
RN 193280-03-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-.beta.-D-xylopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



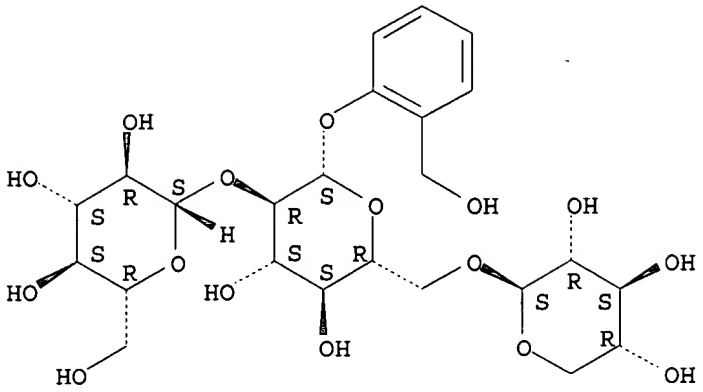
IT **377086-35-6P 377086-36-7P**
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(glycosides of benzyl and **salicyl** alcs. from Alangium chinense)
RN 377086-35-6 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 2-O-.beta.-D-glucopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 377086-36-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl O-.beta.-D-glucopyranosyl-(1.fwdarw.2)-O-[.beta.-D-xylopyranosyl-(1.fwdarw.6)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:560508 CAPLUS
DOCUMENT NUMBER: 135:288062
TITLE: Does excretion of secondary metabolites always involve a measurable metabolic cost? Fate of plant antifeedant salicin in common brushtail possum, Trichosurus vulpecula
AUTHOR(S): McLean, S.; Pass, G. J.; Foley, W. J.; Brandon, S.; Davies, N. W.
CORPORATE SOURCE: School of Pharmacy, University of Tasmania, Hobart, 7001, Australia
SOURCE: Journal of Chemical Ecology (2001), 27(6), 1077-1089
CODEN: JCECD8; ISSN: 0098-0331
PUBLISHER: Kluwer Academic/Plenum Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Salicin was given to 6 brushtail possums in diet for 6 days at 0.05, 0.5, and 1.5% feed wet wt. (mean daily intakes 0.31.+-.0.09, 2.76.+-.0.75, and 6.04.+-.1.12 mmol salicin, resp.). Salicin metabolites were analyzed by HPLC and MS. **Salicyl** alc. glucuronide accounted for 56-64% of urinary metabolites over the 3 doses, salicyluric acid 15-26%, and salicin 10-18%; there were smaller amts. of free (2-4%) and conjugated (0-6%) salicylic acid. The .beta.,2-dihydroxyphenylpropionic acid was a minor metabolite. Hydrolysis of the dietary salicin allowed reconjugation of its aglycon, **salicyl** alc., with a more polar sugar, glucuronic acid, thus enhancing its renal excretion and leading to small net loss of substrates for conjugation and low measurable metabolic costs of excretion.

IT **138-52-3**, Salicin
RL: BPR (Biological process); BSU (Biological study, unclassified); FFD (Food or feed use); BIOL (Biological study); PROC (Process); USES (Uses)
(dietary salicin plant antifeedant compd. intake and metabolic cost of its urinary metabolites excretion in common brushtail possum (Trichosurus vulpecula))
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

SYNTHESIS OF IMIDAZO[1,2-c]PYRIMIDINE DERIVATIVES

Florentina Georgescu,[3] Emilian Georgescu,[3] Paula C. Iuhas,[3] Constantin Draghici," Miron Caproiu,[b]Petru I. Filip[b] a. S. C. *OLTCHIM S. A.-Research Center, 1 Uzinei St., 1000 Ramnicu Valcea, Romania;*
e-mail: sinteze@oltchim. onix. ro
b. Romanian Academy-Center for Organic Chemistry, Spl. Independentei 202B, 77208 Bucharest, Romania

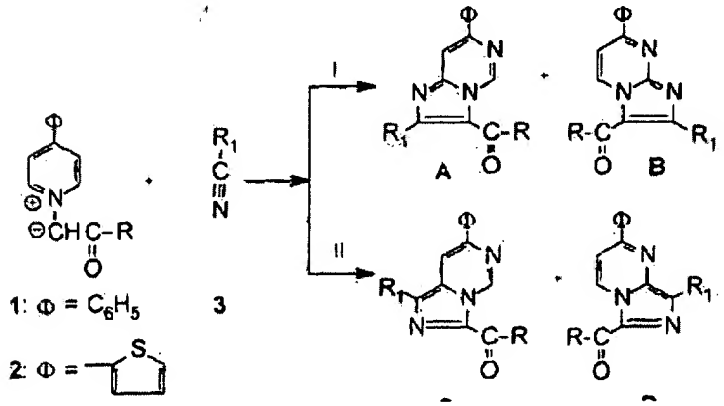
Introduction

Imidazo[1,2-c]pyrimidine derivatives have interesting chemical and biological properties, which raised up numerous studies.[1-4] In this field we are particularly interested in the synthesis of imidazo [1,2-c]pyrimidine derivatives with potential biological activities.

The common methods for the synthesis of imidazo-azines are based on the condensation reactions: the condensation of heterocyclic amines with cc-halocarbonyl compounds[1-3], the reaction of cc-aminoheterocyclic compounds with 1,2-dibromoethane followd by oxidation[4], or the reaction of chloroazines with a-aminoacetaldehyde diethyl acetal[4,5]. An interesting method for the synthesis of imidazo-azines is based on 1,3-dipolar cycloaddition reactions of cycloimmonium-ylides with dipolarophile compounds containing activated carbon-nitrogen triple bond. This method was applied for the synthesis of imidazo[1,2-a]pyridine and imidazo[2,1-b]isoquinoline derivatives by the 1,3-dipolar cycloaddition reactions of pyridinium-and isoquinolinium-ylides with trifluoroacetonitrile[6]. Only one imidazo[1,2-a]pyrimidine, with very poor yield, was obtained by this method. Herein, we present new imidazo[1,2-a]pyrimidine derivatives obtained by 1,3-dipolar cycloaddition reactions of 4-substituted pyrimidinium-ylides with dipolarophile compounds containing activated carbon-nitrogen triple bond such as trifluoroacetonitrile and benzoyl cyanide.

Results and Disscusion

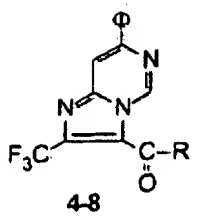
Theoretically, in the [3+2] dipolar cycloaddition reactions of 4-substituted pyrimidinium-ylides with unsymmetrical substituted carbon-nitrogen triple bond compounds the following regioisomers A-C could be obtained (scheme 1).



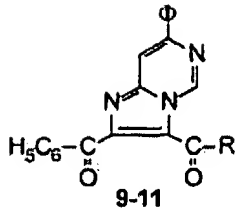
Scheme 1. The four possible regioisomers in the [3+2] dipolar cycloadditions of 4-substituted pyrimidinium-ylides to carbon-nitrogen triple bond compounds.

By the reactions of several 4-substituted pyrimidinium-ylides 1, and respectively 2, to trifluoroacetonitrile **3a** (RpCFs), and respectively benzoyl cyanide 3b (Ri=C_6H_5), only one type of each trifluoromethyl-substituted imidazo[1,2-c]pyrimidines 4-8, respectively benzoyl-substituted imidazo[1,2-c]-pyrimidines 9-11, were obtained (scheme 2). The 4-substituted pyrimidinium-ylides were generated *in situ* from the corresponding quaternary salts in the presence of an acid acceptor such as triethylamine or 1,2-epoxybutane.[7-10]

New prepared 5-trifluoromethyl- and 5-benzoyl-pyrrolo[1,2-c]pyrimidine derivatives 4-11 (scheme 1) were characterised by melting points, IR and NMR spectroscopy. IR and NMR data confirm the A-type structure of the obtained cycloadducts 4-11.



4-8



9-11

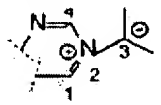
Comp.	o>	R	m.p. (°C)	Yield (%) 4	C_6H_5
C_6H_5	197-198.5	30.2 5	C_6H_5	C_6H_4F(pJ	198-201
29.4 6	C_6H_5	$C_6H_4OCH_3$(p/)	173-176	28.2 7	C_6H_6
$C_6H_4NO_2$(pJ	248-251	34.5 8	2-thienyl	C_6H_3(3,4-OCH_3)2	239-241
30.0 9	C_6H_5	C_6H_5	215-217	29.4 10	C_6H_5
$C_6H_4NO_2$(pJ	242-244	34.2 11	2-thienyl	C_6H_3(3,4-OCH_3)2	230-234
30.6					

Scheme 2. New synthesized imidazo[1,2-c]pyrimidines

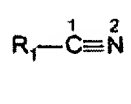
A theoretical study concerning the regiochemistry of cycloaddition reactions of 4-substituted pyrimidinium-ylides as 1,3-dipoles to trifluoroacetonitrile and benzoyl cyanide as dipolarophiles was performed to explain the regioselectivity. We have used the General Theory of Perturbation of the Molecular Frontier Orbitals [1|12].

The energies (eV) of frontier molecular orbitals (HOMO and LUMO), the coefficients of atomic orbital p_z and the total atomic charges (in coulombs) for all the atoms involved in the cycloaddition reactions of pyrimidinium-ylides **1a** and **2a** to trifluoroacetonitrile 3a, respectively benzoyl cyanide 3b, are presented in Table 1.

Table 1. Atomic charges, atomic orbital coefficients and frontier molecular orbital energies of ylides **1a** and **2a,** trifluoroacetonitrile 3a and benzoyl cyanide 3b.



1/2



3

Frontier orbitals	Orbital	Molecule molecular energy (eV)	C-1	N-2	C-3	C-4	
Ylidela	HOMO	-7.78297	+0.33413	+0.07110	-0.65444	+0.33643	<D=C_6H_5,
LUMO	-1.24434	+0.26000	-0.44268	-0.30670	+0.19343	R=C_6H_5	Q
-0.160	+0.142	-0.404	-0.082	Ylide2a	HOMO	-7.7755	+0.3084
+0.0699	-0.6209	+0.3234	<X>=2-thienyl,	LUMO	-1.3153	-0.1736	+0.4041 -
0.2969	-0.2226	R=C_6H_4(3,4-	Q		-0.135	+0.142	-0.412 -
0.104	$OCH_3)_2$	3a	HOMO	-14.18754	+0.34271	-0.38373	(Ri=CF_3) LUMO
+0.35250	-0.26350	+0.27280	Q		-0.213	+0.079	3b HOMO -
10.37269	-0.00027	+0.00179	(R^CeHsCO)	LUMO	-1.03313	-0.14256	+0.24799 Q
-0.183	+0.011						

The pyrimidinium-ylides, trifluoroacetonitrile and benzoyl cyanide considered geometries and all data presented in table 1 were calculated by AM1 method [13], using the HyperChem Program [14]. The correlation diagrams (figure 1) between HOMO and LUMO orbitals of ylides **1a**, respectively **2a,** and of trifluoroacetonitrile **3a,** respectively benzoyl cyanide **3b,** have been elaborated using

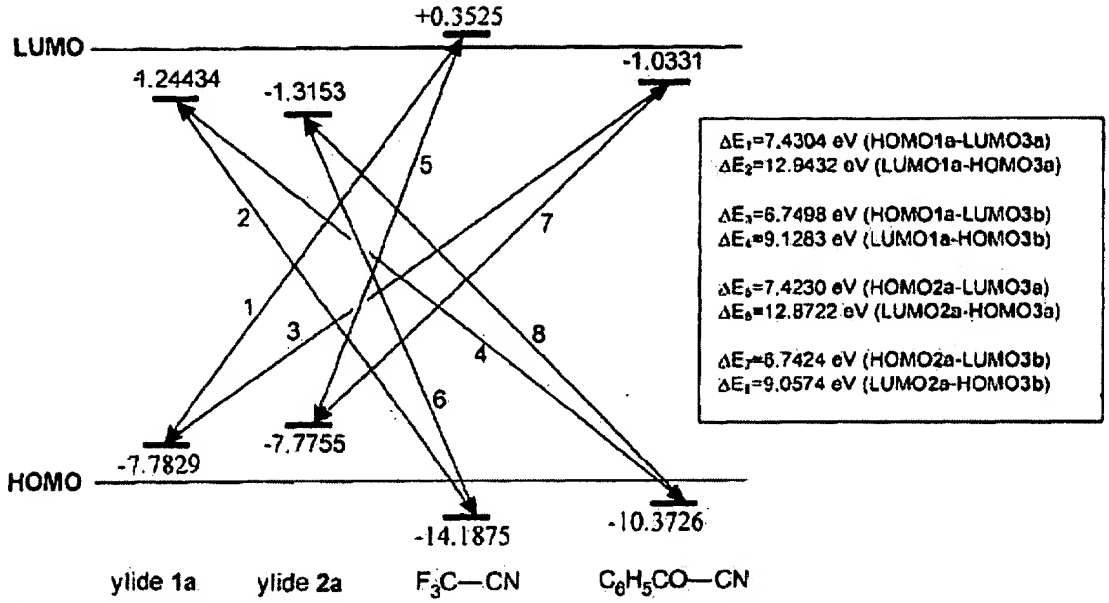


Figure 1. Correlation diagrams

According to the orbital correlation diagrams presented in figure 1, the interactions HOMO ylide - LUMO dipolarophile are characterised by the lowest interaction energies (AE_1=7.4304 eV for the ylide 1a-trifluoroacetonitrile and AE_3=6.7498 eV for the ylide 1a-benzoyl cyanide, respectively AE_5=7.4230 eV for the ylide 2a-trifluoroacetonitrile and AE_7=6.7424 eV for the ylide 2a-benzoyl cyanide). All these cycloaddition reactions are HOMO-controlled in respect to the ylide. This means that in the reaction ylide (donor) - dipolarophile (acceptor), under orbital or charge control, the most likely interaction will take place between C_3 atom of the ylide and nitrogen atom of the trifluoroacetonitrile, respectively benzoyl cyanide (figure 2).

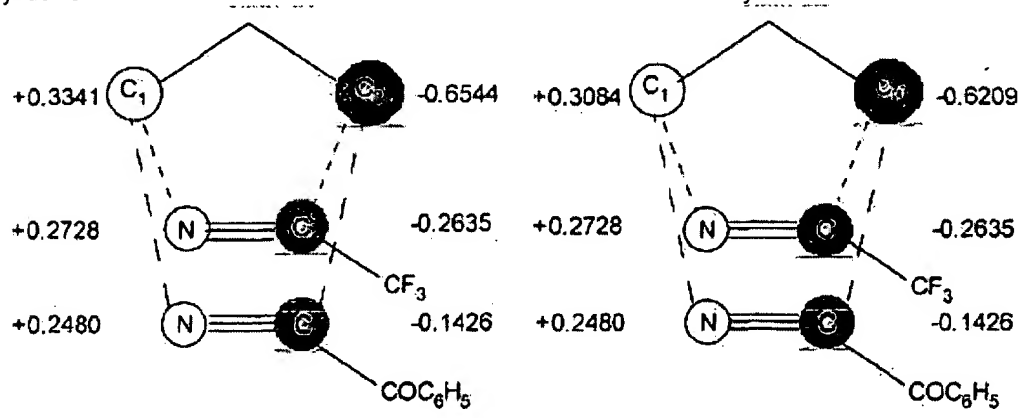


Figure 2. Graphical representation of the interaction between the frontier molecular orbitals

Taking into account that in figure 2 the atomic orbital coefficients have the same signs, the formation of A-type cycloadduct is allowed. Thus, in the case of pyrimidinium-ylides, the new bound will be realised between the ylidic carbon and the nitrogen atom from the carbon-nitrogen triple bound compounds, affording imidazo[1,2-c]pyrimidine derivatives 4-11 with A-type structures.

Conclusion

New 2,3-disubstituted imidazo [1,2-c]pyrimidine derivatives 4-11 were obtained by 1,3-dipolar cycloaddition reactions of several 4-substituted pyrimidinium-ylides, as 1,3-dipols, with activated triple bond carbon-nitrogen compounds such as trifluoroacetonitrile and benzoyl cyanide.

Analysis of all data leads to the conclusion that the [3+2} dipolar cycloaddition reactions of 4-substituted pyrimidinium-ylides, to trifluoroacetonitrile, respectively benzoyl cyanide, are regioselective. The reactions are HOMO controlled by ylides and only one regioisomer is formed, the one in which the ylide carbanion makes the new bound with the nitrogen atom from trifluoroacetonitrile, respectively benzoyl cyanide. Thus, the theoretical and experimental data are in accordance with each other.

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